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Published in:
Journal of Chemical & Engineering Data

DOI:
10.1021/je00011a037

Publication date:
1993

Diffusion Coefficients of Several Aqueous Alkanolamine Solutions

Erwin D. Snijder, Marcel J. M. te Riele, Geert F. Versteeg,* and W. P. M. van Swaaij

Department of Chemical Engineering, Twente University of Technology, P.O. Box 217, 7500 AE Enschede, The Netherlands

The Taylor dispersion technique was applied for the determination of diffusion coefficients of various systems. Experiments with the system KCl in water showed that the experimental setup provides accurate data. For the alkanolamines monoethanolamine (MEA), diethanolamine (DEA), methyldiethanolamine (MDEA), and di-2-propanolamine (DIPA), correlations for the diffusion coefficient as a function of temperature at different concentrations are given. A single relation for every amine has been derived which correlates the diffusion coefficients as a function of temperature and concentration. The temperature was varied between 298 and 348 K, and the concentration between 0 and 4000–5000 mol/m^3. Furthermore, a modified Stokes–Einstein relation is presented for the prediction of the diffusion coefficients in the alkanolamines in relation to the viscosity of the solvent and the diffusion coefficient at infinite dilution. The diffusion coefficients at low concentrations are compared with some available relations for the estimation of diffusion coefficients at infinite dilution, and it appears that the agreement is fairly good.

1. Introduction

Estimation methods for diffusion coefficients have always had much attention in the literature (*1–6*). Most of the derived relations are well applicable for ideal systems at low concentrations; however, in more concentrated systems usually large errors arise. Reliable dimensioning of process equipment requires accurate knowledge of diffusion coefficients. Sherwood relations contain diffusion coefficients in order to estimate mass transfer coefficients, which are used in design techniques for absorption, extraction, and distillation processes. In absorption processes of acid gases (H_2S, CO_2, COS) in alkanolamine solutions diffusion coefficients are used for the calculation of the mass transfer rate (see, e.g., ref 7). Obviously, rather than estimating the diffusion coefficients, more precise data can be obtained by measuring the values in the actual system.

Nowadays many different techniques are known. Relatively old is the use of a diaphragm cell (Stokes (*8*)). Disadvantages, however, are the very long measuring time and the need for calibration of the cell with a known system. Optical methods (*9, 10*) are fast, but require special equipment. For gas–liquid diffusion coefficients the stationary bubble method (*11*) or the laminar jet (*12*) can be used. A technique which is frequently used to date is the Taylor dispersion method (*13–17*). Taylor (*18*) has demonstrated that axial dispersion takes place when a solute is introduced in a solvent flowing slowly through a long capillary tube. This is caused by the combination of axial laminar convection and radial diffusion. By solving the mass balance for such a system, Taylor was able to relate the diffusion coefficient to the measured axial dispersion coefficient. The method is relatively fast, and there is no need for calibration with a well-known system.

The Taylor dispersion method has been used in the present study to measure diffusion coefficients of several alkanolamine solutions in water as well as KCl in water.

2. Theory

In the Taylor dispersion method a pulse of concentrated solute is injected in the solvent. Owing to the laminar velocity profile in the tube, the shape of the pulse becomes parabolic initially. Diffusion tends to decrease the concentration gradients, resulting in a spreading out of the solute. Equation 1 describes the process of instationary fluid flow through a

$$\frac{\partial C}{\partial t} = D\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right) + \frac{\partial^2 C}{\partial x^2}\right) - 2u\left(1 - \frac{r^2}{R^2}\right)\frac{\partial C}{\partial x} \quad (1)$$

straight tube under laminar conditions. Taylor (*18, 19*) showed that under certain conditions the diffusion process can be regarded as axial dispersion of solute material around a plane which moves with average velocity u through the tube. Aris (*20*) evaluated the diffusion equation (1) by calculating the different moments and derived that the dispersion coefficient can be calculated according to

$$K = u^2R^2/48ID + D \quad (2)$$

In practice, some important restrictions on the experimental conditions must be considered. Alizadeh *et al.* (*21*) gave a complete review on the determination of diffusion coefficients with the Taylor dispersion method. They suggested using a statistical method, and the diffusion coefficient should then be calculated according to

$$D = R^2\bar{t}_{id}/24{\sigma_{id}}^2 \quad (3)$$

Corrections on the ideal average residence time and variance are given for a non-δ-Dirac pulse injection, finite detection volume, and deviations in tube geometry. Another important phenomenon is the development of secondary flow. This is caused by gravitational forces in the case of flow through a curved tube (*22, 23*) or by differences in density between the solvent and solute (*24–26*). All these considerations lead to a well-defined range for the experimental conditions under which the Taylor dispersion technique is applicable for the determination of diffusion coefficients.

Whether these conditions are rigorous enough can be evaluated either experimentally (system with well-known diffusion coefficient) or by solving the total diffusion equation numerically. Among others, this has been demonstrated by Snijder (*27*). His results, which have been applied in the present work, agree very well with the restrictions as proposed by Alizadeh *et al.* (*21*).

3. Results

3.1. Introduction. With the Taylor dispersion technique the diffusion coefficients of the following systems were

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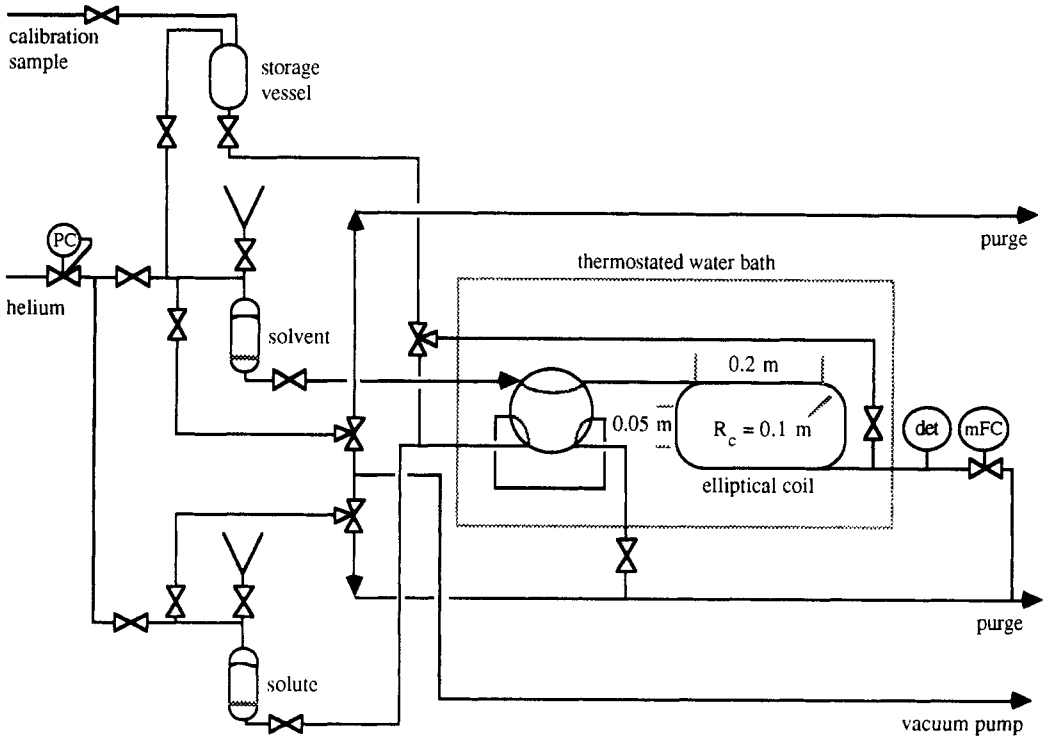

Figure 1. Experimental setup.

examined: (1) KCl in water; (2) monoethanolamine (MEA) in aqueous MEA solutions; (3) diethanolamine (DEA) in aqueous DEA solutions; (4) methyldiethanolamine (MDEA) in aqueous MDEA solutions; (5) di-2-propanolamine (DIPA) in aqueous DIPA solutions. The first system was used to check whether accurate values for the diffusion coefficients can be obtained when the experimental restrictions are taken into account. As mentioned before, diffusion coefficients of alkanolamine systems are necessary for the design of gas-treating processes, which are of large industrial importance. Until now only a very limited amount of experimental data on diffusion coefficients was available for concentrated amine solutions. Thomas and Furzer (*9*) and Hikita *et al.* (*28*, *29*) have presented values for different amines and concentrations. Yet they carried out their measurements at 298 K only, and the maximum concentration in their work was still somewhat below the values being used in industrial treating processes. In this work their data are extended to higher concentrations and a temperature range of 298–348 K.

The experimental setup which has been used is shown schematically in Figure 1. Two glass storage vessels containing solute and solvent are kept at a constant helium pressure by means of a precision pressure control valve. Regulating the flow after the detector (differential refractometer, Varian RI 4) with a mass flow controller (Rosemount Flowmega 5881) yields a complete pulsation-free and constant flow throughout the experiment. Introduction of a solute pulse is performed by switching the helium-actuated six-way valve (0.1–0.2-s switching time). The capillary tube is elliptically coiled and is placed in a water bath which can be kept at the desired temperature within 0.1 K. Calibration of the refractometer is carried out by passing reference samples directly through the refractometer. The dimensions of the tube and the experimental conditions are given in Table I.

The method as presented by Baldauf and Knapp (*14*) is followed for the conversion of the collected data to concentrations. First the drift in the base line of the refractometer (generally this is only very little) is subtracted from the response, after which the concentration is calculated using a calibration function. The method of Levenberg and Marquardt (*30*) has been used for fitting the concentration curve

Table I. Dimensions of the Setup and Experimental Conditions

dimensions	flow conditions
L_c = 15.085 m	u = 2.5–5 mm/s
R = 5.565 × 10^{-4} m	Pe = 1000–8000
R_c = 0.10 m	τ = 10–40
V_c = 1.47 × 10^{-5} m^3	
V_{inj} = 8.76 × 10^{-8} m^3	
V_{det} = 8 × 10^{-9} m^3	

$C_m(x=L,t)$ on eq 3; initial guesses for N_{inj}, u, and K have been obtained by means of a statistical procedure (*15*).

$$C_t = \sum C_m(x=L,t)\,\Delta t \qquad N_{inj} = uSC_t$$

$$\bar{t} = (1/C_t)\sum C_m(x=L,t)t\,\Delta t \qquad u = L/\bar{t} \qquad (4)$$

$$\sigma_t^2 = (1/C_t)\sum C_m(x=L,t)(t-\bar{t})^2\,\Delta t \qquad K = L^2\sigma_t^2/2\bar{t}^3$$

Here N_{inj} is the amount of moles in the injected pulse in excess of those already present in the solvent. It must be noted, however, that the injected pulse of the solute usually consisted of a solution and not of the pure compounds. Since the concentration of the solution decreases during the dispersion process, an average value has to be determined. Alizadeh *et al.* (1980) called it the reference concentration (C_{ref}) and gave the following equation:

$$C_{ref} = C_{solv} + \frac{N_{inj}(5/16 - 1/8\pi^{1/2})}{\pi R^2(2K\bar{t})^{1/2}} \qquad (5)$$

3.2. KCl–Water, a Test Experiment. The determination of diffusion coefficients of KCl in water was carried out in order to investigate the influence of secondary flow due to the coiling of the tube. At 298 K and at various liquid velocities the diffusion coefficient and the reference concentration have been calculated from the fitted dispersion coefficient. Figure 2 shows the influence of $(De)^2Sc$ on D/D_{lit}; the comparison with the literature data is given in Table II. Below a critical value of about 180 for $(De)^2Sc$ the measured diffusion coefficients are almost identical to the literature value. The

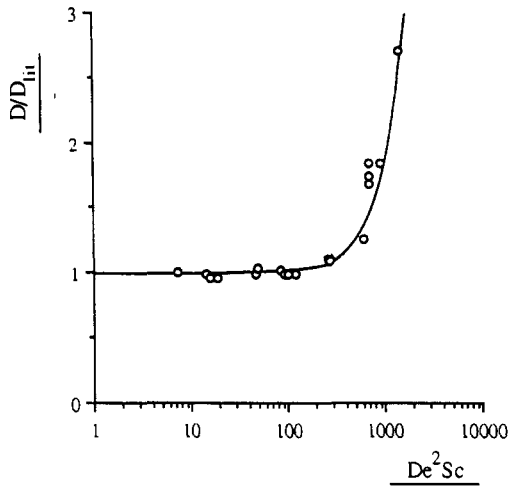

Figure 2. Influence of $(De)^2Sc$ on the deviation of the diffusion coefficient of KCl in water at 298 K.

Table II. Diffusion Coefficients of KCl in Water

T/K	c_{ref}/(mol/m³)	$D \times 10^9$/(m²/s)	ref
298	5.4	1.89	present work
298	3.0	1.96	34
298	5.0	1.95	34
298	7.0	1.95	34
308	3.6	2.50	present work
308	100	2.37	35
323	5.0	3.41	present work
323	99.1	3.07	35

Table III. Diffusion Coefficients, Densities, and Viscosities of Aqueous MEA Solutions

T/K	c/(mol/m³)	$D \times 10^9$/(m²/s)	ρ/(kg/m³)	$\eta \times 10^3$/(Pa·s)
298.0	43	1.12	996.9	0.89
297.9	1012	1.00	999.1	1.07
297.9	2009	0.91	1001.6	1.31
298.1	5012	0.69	1010.0	2.31
308.0	49	1.39	994.1	0.73
308.0	1014	1.28	995.1	0.85
308.0	2012	1.17	998.1	1.02
308.0	5011	0.93	1006.0	1.78
318.0	55	1.75	990.4	0.60
318.0	1015	1.59	992.1	0.68
318.1	2017	1.45	994.1	0.79
318.1	5016	1.18	1001.0	1.22
333.0	58	2.26	983.3	0.47
332.9	1020	2.10	984.8	0.53
333.0	2016	1.99	986.5	0.60
333.0	5015	1.64	992.5	0.90

critical $(De)^2Sc$ is much higher than 20, which was proposed by Alizadeh *et al.* (*21*). The value 20 holds, however, for a circular coil, whereas in this work an elliptical coil has been used. Experiments were also carried out at higher temperatures, and these are listed in Table II, together with available literature data.

The conclusion from these experiments is that, in the setup as applied in the present investigations, the agreement between measured and literature diffusion coefficients is good as long as $(De)^2Sc$ is below 180. For every new system it was checked whether this restriction holds.

3.3. Alkanolamine Solutions. 3.3.1. MEA in Aqueous MEA Solutions. The diffusion coefficients of MEA in aqueous MEA solutions were determined for concentrations between about 40 and 5020 mol/m³ and temperatures between 298 and 333 K. The results (average of 3–4 data points) are listed in Table III. Values for the viscosities and densities of the solutions are obtained from the information as presented by Littel *et al.* (*31*). For this system the critical $(De)^2Sc$ number is again about 180; at higher flow velocities the fitted diffusion coefficients appeared to increase. All data points were determined at conditions with $(De)^2Sc \leq 120$.

Table IV. Literature Data on Diffusion Coefficients of Various Alkanolamine Solutions at 298 K

c/(mol/m³)	$D \times 10^9$/(m²/s)	system	ref
47	1.15	MEA	28
1070	0.984	MEA	28
1980	0.910	MEA	28
670	1.02	MEA	9
1670	0.852	MEA	9
3340	0.511	MEA	9
51	0.808	DEA	28
1040	0.617	DEA	28
2210	0.486	DEA	28
1050	0.464	DEA	9
2100	0.382	DEA	9
4190	0.281	DEA	9
50	0.720	DIPA	29
1020	0.488	DIPA	29
2040	0.338	DIPA	29
3010	0.199	DIPA	29

Table IV lists literature data; the experimental values correspond very well with the data as reported by Hikita *et al.* (*28*). The results as presented by Thomas and Furzer (*9*) appear to be too low. Correlations for the temperature dependency of the diffusion coefficients have been obtained at average amine concentrations:

$$C = 51 \text{ mol/m}^3 \qquad D = 1.006 \times 10^{-6} \exp(-2028.9/T)$$

$$C = 1015 \text{ mol/m}^3 \qquad D = 1.137 \times 10^{-6} \exp(-2094.3/T)$$

$$C = 2014 \text{ mol/m}^3 \qquad D = 1.423 \times 10^{-6} \exp(-2190.1/T) \quad (6)$$

$$C = 5014 \text{ mol/m}^3 \qquad D = 2.487 \times 10^{-6} \exp(-2436.7/T)$$

The influence of temperature and concentration on the diffusion coefficient has been fitted with a single relation which provides the diffusion coefficient within 5% tolerance for the complete temperature and concentration range. The Nelder–Mead method (*30*) was applied for the minimization of a χ^2 function which is defined according to

$$\chi^2 = \sum_i (\ln(D_i) - (A_1 + A_2/T_i + A_3 C_i))^2 \quad (7)$$

Using all data points and fitting A_1, A_2, and A_3 yield

$$\ln(D) = -13.275 - 2198.3/T - 7.8142 \times 10^{-5} C \quad (8)$$

$$\text{for} \quad 43 \leq C \leq 5016 \text{ mol/m}^3$$

$$298 \leq T \leq 333 \text{ K}$$

Figure 3 depicts a parity plot of the calculated versus experimental diffusion coefficients.

3.3.2. DEA in Aqueous DEA Solutions. The data for DEA diffusivities are treated in exactly the same way as those for MEA. On the basis of the velocity influence on the fitted diffusion coefficient, it has been concluded that the critical $(De)^2Sc$ was lower for this system (about 100). The experiments were carried out at flow velocities with $(De)^2Sc \leq 70$. Table V gives the determined values for the concentration range 10–4010 mol/m³ and the temperature range 298–348 K. Viscosity and density data at 298 K were provided by Versteeg and van Swaaij (*32*), at 308, 318, and 333 K by Littel *et al.* (*31*). The densities and viscosities at 4000 mol/m³ were measured. Table IV lists some available literature results at 298 K. The agreement between the diffusion data as presented in this work and by Hikita *et al.* (*28*) is less than for MEA; the results of Thomas and Furzer (*9*) are again

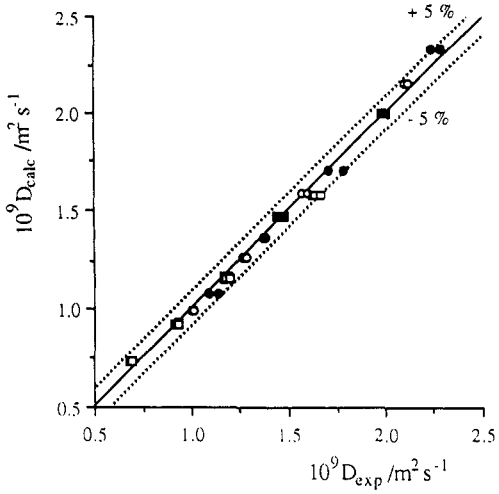

Figure 3. Diffusion coefficients for MEA solutions determined experimentally and calculated with eq 11: (●) 51 mol/m^3, (○) 1015 mol/m^3, (■) 2014 mol/m^3, (□) 5014 mol/m^3.

Table V. Diffusion Coefficients, Densities, and Viscosities of Aqueous DEA Solutions

T/K	c/(mol/m^3)	$D \times 10^{-9}$/(m^2/s)	ρ/(kg/m^3)	$\eta \times 10^3$/(Pa·s)
298.0	10	0.84	997.1	0.88
298.0	1007	0.66	1009.6	1.28
298.0	1984	0.53	1021.6	1.89
298.0	4010	0.34	1046.0	5.31
308.0	10	1.06	994.1	0.74
308.0	1008	0.85	1006.1	1.00
308.0	1989	0.70	1017.6	1.50
308.0	4011	0.45	1040.6	3.74
318.0	11	1.33	990.3	0.60
317.9	1009	1.08	1001.8	0.83
318.0	1991	0.89	1013.0	1.14
318.1	4011	0.61	1035.6	2.74
333.0	12	1.76	983.3	0.47
333.1	1010	1.44	992.8	0.61
333.0	1995	1.23	1004.6	0.85
333.0	4012	0.86	1026.9	1.90
348.0	9	2.26	974.6	0.37
348.2	1012	1.90	982.4	0.47
348.0	2000	1.64	1002.7	0.63
348.0	4013	1.18	1017.9	1.41

rather low. The following relations have been obtained:

$$C = 10 \text{ mol/m}^3 \qquad D = 0.8308 \times 10^{-6} \exp(-2052.5/T)$$

$$C = 1009 \text{ mol/m}^3 \qquad D = 0.9331 \times 10^{-6} \exp(-2157.5/T)$$

$$C = 1992 \text{ mol/m}^3 \qquad D = 1.397 \times 10^{-6} \exp(-2343.4/T) \quad (9)$$

$$C = 4011 \text{ mol/m}^3 \qquad D = 2.150 \times 10^{-6} \exp(-2610.0/T)$$

An equation which fits all data points within 7% accuracy reads

$$\ln(D) = -13.268 - 2287.7/T - 19.699 \times 10^{-5} C \quad (10)$$

$$\text{for} \quad 9 \le C \le 4013 \text{ mol/m}^3$$

$$298 \le T \le 348 \text{ K}$$

3.3.3. MDEA in Aqueous MDEA Solutions. The average results for MDEA solutions are listed in Table VI; the temperature was varied between 298 and 348 K and the concentration between about 10 and 4000 mol/m^3. The viscosity data were obtained from Versteeg and van Swaaij (*32*) (the values at 4000 mol/m^3 have been measured). All densities were measured as well. The experiments were

Table VI. Diffusion Coefficients, Densities, and Viscosities of Aqueous MDEA Solutions

T/K	c/(mol/m^3)	$D \times 10^{-9}$/(m^2/s)	ρ/(kg/m^3)	$\eta \times 10^3$/(Pa·s)
298.0	8	0.79	996.8	0.90
298.0	1004	0.61	1007.3	1.30
298.0	2008	0.46	1018.3	1.97
298.0	4003	0.25	1039.4	7.06
308.0	8	1.00	994.0	0.73
308.0	1006	0.78	1003.8	1.02
308.0	2009	0.60	1014.0	1.49
308.0	4004	0.35	1033.3	4.86
318.0	11	1.26	990.3	0.61
318.0	1007	1.00	999.8	0.84
317.8	2010	0.76	1009.0	1.18
318.0	4005	0.47	1027.0	3.46
333.0	11	1.69	983.2	0.48
333.0	1010	1.32	992.1	0.63
333.0	2011	1.06	997.5	0.87
333.1	4007	0.69	1013.2	2.30
348.0	8	2.18	975.0	0.37
348.0	1012	1.72	983.1	0.48
348.0	2013	1.40	991.1	0.62
348.0	4010	0.96	1005.3	1.61

Table VII. Diffusion Coefficients, Densities, and Viscosities of Aqueous DIPA Solutions

T/K	c/(mol/m^3)	$D \times 10^{-9}$/(m^2/s)	ρ/(kg/m^3)	$\eta \times 10^3$/(Pa·s)
298.0	9	0.71	996.8	0.89
298.0	1004	0.47	1004.7	1.64
298.0	2004	0.33	1014.0	3.21
298.0	3005	0.21	1020.9	7.12
308.0	8	0.81	994.0	0.72
308.0	1005	0.57	1002.4	1.36
308.0	2004	0.37	1012.2	2.83
308.0	3006	0.30	1014.8	4.37
318.0	9	1.14	990.3	0.59
318.0	1006	0.70	999.1	1.08
318.0	2006	0.50	1006.9	1.96
318.0	3008	0.40	1009.4	2.87
333.0	9	1.53	983.2	0.46
333.0	1006	0.88	994.4	0.87
333.0	2006	0.64	1001.4	1.50
333.0	3010	0.59	999.7	2.06
348.0	9	1.99	975.0	0.37
348.0	1007	1.17	987.1	0.66
348.0	2007	0.85	993.1	1.08
348.0	3012	0.81	988.8	1.16

carried out at $(De)^2Sc \le 75$; the following relations have been obtained:

$$C = 9 \text{ mol/m}^3 \qquad ID = 0.9526 \times 10^{-6} \exp(-2112.9/T)$$

$$C = 1008 \text{ mol/m}^3 \qquad D = 0.8096 \times 10^{-6} \exp(-2139.1/T)$$

$$C = 2010 \text{ mol/m}^3 \qquad D = 1.098 \times 10^{-6} \exp(-2316.6/T) \quad (11)$$

$$C = 4006 \text{ mol/m}^3 \qquad D = 2.866 \times 10^{-6} \exp(-2781.2/T)$$

An equation which fits all data points within 9% accuracy reads

$$\ln(D) = -13.088 - (-2360.7/T) - 24.727 \times 10^{-5} C \quad (12)$$

$$\text{for} \quad 8 \le C \le 4010 \text{ mol/m}^3$$

$$298 \le T \le 348 \text{ K}$$

3.3.4. DIPA in Aqueous DIPA Solutions. The measured diffusion coefficients for several DIPA solutions are listed in Table VII; the concentration was varied between about 10 and 3012 mol/m^3. Available literature data (*29*) are given in Table IV; at comparable concentrations the agreement is very good. Again, the viscosities are calculated with

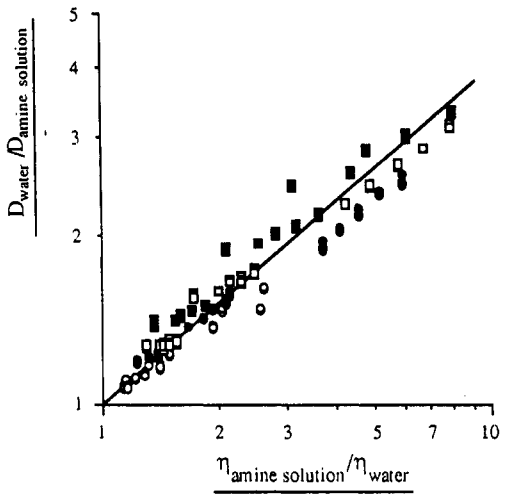

Figure 4. Stokes–Einstein plot of the diffusion coefficient against viscosity for several aqueous alkanolamine solutions: (○) MEA, (●) DEA, (□) MDEA, (■) DIPA.

information as presented by Versteeg and van Swaaij (*32*). All densities have been measured. The experiments were carried out at $(De)^2Sc \leq 85$; equations for the diffusion coefficients at average concentrations are given below:

$$C = 9\ \text{mol/m}^3 \qquad D = 0.9294 \times 10^{-6} \exp(-2136.6/T)$$

$$C = 1006\ \text{mol/m}^3 \qquad D = 1.017 \times 10^{-6} \exp(-2283.4/T)$$

$$C = 2005\ \text{mol/m}^3 \qquad D = 1.120 \times 10^{-6} \exp(-2422.0/T) \quad (13)$$

$$C = 3009\ \text{mol/m}^3 \qquad D = 2.120 \times 10^{-6} \exp(-2734.2/T)$$

An equation which fits all data points within 6% accuracy reads

$$\ln(D) = -13.072 - (-2398.8/T) - 34.660 \times 10^{-5} C \quad (14)$$

$$\text{for} \quad 8 \leq C \leq 3012\ \text{mol/m}^3$$

$$298 \leq T \leq 348\ \text{K}$$

3.3.5. Discussion on the Amine Measurements. It was evaluated whether D_0/D and $\eta_{amine\ solution}/\eta_{water}$ can be correlated according to a modified Stokes–Einstein relation (*32*). For the diffusion coefficients at infinite dilution (D_0), the measured values at low concentrations were taken. All data points of the four alkanolamine solutions are presented in Figure 4. It appears that the relation as proposed by Versteeg and van Swaaij (*32*) at 298 K can be extended to a wider range of concentrations and temperatures:

$$\frac{D_0}{D} = \left(\frac{\eta_{amine\ solution}}{\eta_{water}}\right)^{0.6} \quad (15)$$

The difference between the value as calculated with eq 15 and the experimental value is at average 7% and upto a maximum of 25% for the solutions with the highest concentrations. Consequently, the relation can be used to obtain a fairly accurate estimate for the diffusion coefficient of an alkanolamine, provided that the viscosity and D_0 are available. Measuring the viscosity is generally less complicated than the determination of the diffusion coefficient. A value for D_0 can be found using correlations of, e.g., Othmer and Thakar (*33*), Scheibel (*1*), Wilke and Chang (*2*), and Hayduk and Laudie (*5*).

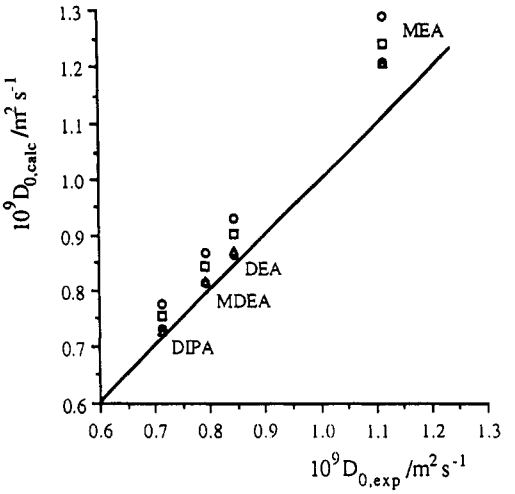

Figure 5. Parity plot of calculated versus experimental diffusion coefficients at infinite dilution: (○) Wilke–Chang, (●) Scheibel, (□) Hayduk, (△) Othmer–Thakar.

Table VIII. Errors between Experimental and Estimated Values for the Diffusion Coefficients at Infinite Dilution

		average error (%)				
system	T/K	Wilke–Chang	Scheibel	Hayduk–Laudie	Othmer–Thakar	Wilke–Chang[a]
MEA	298–333	18.6	11.1	23.5	9.0	10.6
DEA	298–348	11.8	4.2	19.8	2.2	4.2
MDEA	298–348	10.1	2.9	18.0	2.4	5.2
DIPA	297–348	8.2	2.0	16.3	2.8	0.9
average		12.2	5.1	19.4	4.1	5.2

[a] Modified Wilke–Chang equation.

These relations have been tested, including the modification on the Wilke–Chang equation as proposed by Hayduk and Laudie who suggested using 2.26 as the association parameter instead of 2.6. The required molar volumes of the alkanolamines are obtained with the method of LeBas as described by, e.g., Wilke and Chang. The relations of Scheibel, Othmer, and Thakar and the modified Wilke–Chang equation yielded almost the same value for the diffusion coefficient. In Figure 5 these estimated diffusion coefficients are plotted against the experimentally determined values at low concentrations and at a temperature of 298 K. Table VIII lists the average errors between the measured diffusion coefficients and the estimated values according to the correlations mentioned above. The measured values are somewhat lower than the values as estimated with the given correlations, which might be attributed to a too low molar volume. The best results have been obtained with the modified Wilke–Chang equation and the relation of Othmer and Thakar.

4. Conclusions

It has been demonstrated that the Taylor dispersion technique is an accurate method for the determination of diffusion coefficients, provided that certain restrictions on the experimental conditions are fulfilled. With this method diffusion coefficients of MEA, DEA, MDEA, and DIPA in the corresponding aqueous alkanolamine solutions have been measured. The diffusion coefficients have been correlated as a function of temperature and concentration. Moreover, it was shown that the modified Stokes–Einstein relation, $D_0/D = (\eta_{amine\ solution}/\eta_{water})^{0.6}$, proposed by Versteeg and van Swaaij (*32*), can be extended to higher alkanolamine concentrations and temperatures. Several equations for the estimation of the diffusion coefficients at infinite dilution were evaluated. The best results have been obtained with the equations of Wilke and Chang (modified according to Hayduk and Laudie (*5*)) and Othmer and Thakar (*33*).

Acknowledgment

We acknowledge G. B. Broeze and M. J. W. Frank for their contribution to the numerical and experimental work and K. van Bree, S. Kuipers, W. Leppink, and A. H. Pleiter for their technical support. J. A. M. Kuipers and F. P. H. van Beckum are acknowledged for their advice on the numerical method.

Notation

C	concentration, mol/m^3
D	diffusion coefficient, m^2/s
De	Dean number, Re/$\omega^{1/2}$
K	Taylor–Aris dispersion coefficient, m^2/s
L	length of the tube, m
L'	mixing length, m
N	number of moles, mol
Pe	Péclet number, $2uR/D$
R	radius of the tube, m
r	radial coordinate, m
Re	Reynolds number, $2\rho uR/\eta$
S	area of the tube, m^2
Sc	Schmidt number $\eta/(\rho D)$
T	temperature, K
t	time, s
u	average flow velocity, m/s
x	axial coordinate, m
x_1	transformed axial coordinate ($x - ut$), m

Greek Symbols

δL	half pulse width, m
η	dynamic viscosity, Pa·s
ρ	density, kg/m^3
$\sigma^2(t)$	variance, m^2
τ	dimensionless time, Dt/R^2
ω	radius ratio, R_c/R

Subscripts/Superscripts

c	coil
calc	calculated
crit	critical value
det	detector
exp	experimental
id	under ideal conditions
inj	injected
m	mean value
0	at inlet conditions
ref	reference
solv	solvent
t	tracer

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Received for review March 19, 1993. Accepted April 18, 1993. These investigations were supported by the Foundation for Chemical Research in the Netherlands (SON) and by DSM.